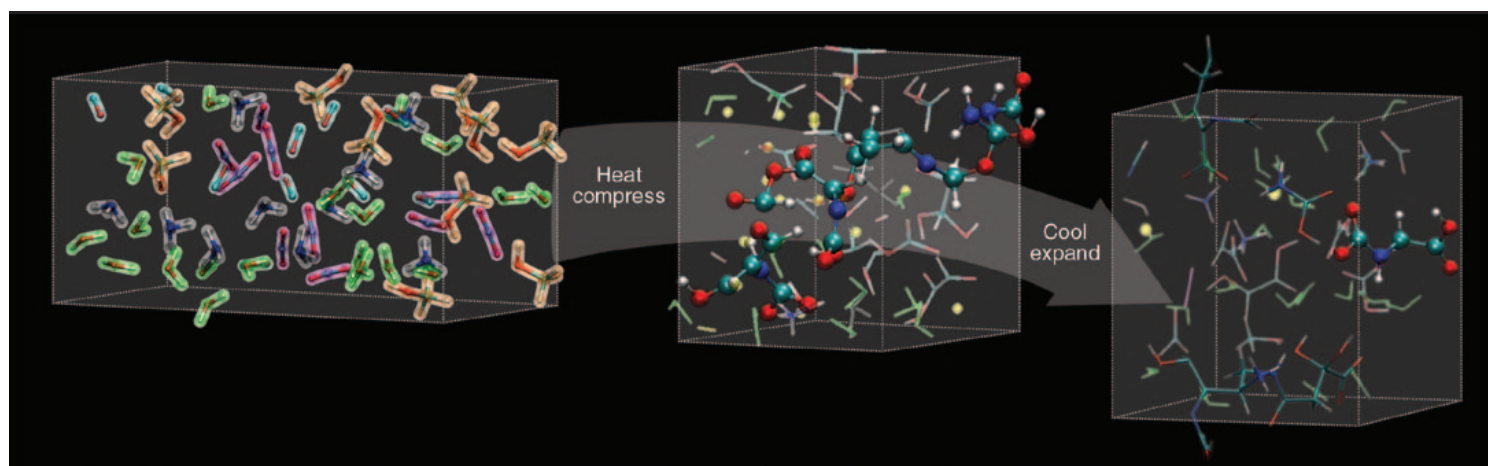


Life from Outer Space

BACK before life as we know it began on Earth—3 to 4 billion years ago—comets were regular visitors. Because of the high temperatures generated when a comet directly strikes Earth, scientists have thought it unlikely that such impacts left much behind, certainly not the materials that would bring about the origins of life. But computational simulations by a team at Lawrence Livermore indicate that a different outcome is possible. “Comets contain methanol, water, carbon dioxide, carbon monoxide, and ammonia, among a few other molecules, which are precursors to amino acids,” says Nir Goldman, a physical chemist in the Laboratory’s Physical and Life Sciences Directorate. “If a comet struck Earth at a low enough angle, shock waves within it could have yielded amino acids—the building blocks of life—and left them behind.”

Origins-of-life research initially focused on the production of amino acids from organic materials already present on Earth. Although the actual composition of the planet’s early atmosphere is unknown, the current view is that it consisted primarily of carbon dioxide, nitrogen, and water. Shock-heating experiments and calculations show that the organic molecules

In this rendering, a prototypical comet composed of methanol, water, carbon monoxide, ammonia, and carbon dioxide crashes into Earth. (Rendering by Kwei-Yu Chu.)



Computer simulations show (left) the molecular makeup of a comet before it strikes Earth, (middle) the long chains of carbon–nitrogen bonds created by the heating and compression that occur on impact, and (right) a long chain breaking apart to form complexes that contain glycine, a protein-building amino acid.

required to produce amino acids could not be synthesized in such an environment, leaving researchers with the question: where did amino acids—and the proteins and larger life forms that grow from them—come from?

Life on Ice

Comets, roaming through the freezing universe, are icy objects, ranging from less than 2 to about 56 kilometers in diameter, on average. As they pass through Earth's atmosphere, they are heated externally but remain cool inside. When a comet hits Earth, the resulting shock wave generates sudden, intense pressures and temperatures up to tens of thousands of kelvins. Such extreme conditions could affect chemical reactions within the comet before it interacts with the ambient planetary environment. The consensus had been that the intense heating from the impact would destroy any potential life-building molecules.

To study comet impacts in more detail, the Livermore team, which includes Laurence Fried, William Kuo, Amitesh Maiti, and former Laboratory employee Evan Reed, now at Stanford University, conducted computer simulations in which a comet strikes Earth at an angle of up to 24 degrees from the horizon. Results show that a glancing blow such as this one would generate significantly lower temperatures. "Under those conditions, organic materials could potentially be synthesized within the comet's interior during shock compression," says Goldman, who leads the project team. "Once the compressed material expands, stable amino acids might survive interactions with the

planet's atmosphere or ocean. These processes could result in concentrations of prebiotic organic species from materials that originated in the outer regions of space."

Amino Acid Synthesis Revealed

The team explored amino acid synthesis in a shock-compressed astrophysical ice mixture using quantum molecular-dynamics simulations. Quantum simulations can offer an accurate reproduction of shock compression, greatly facilitating experimental design and theory. These calculations predict activity at the electronic scale, allowing scientists to examine processes occurring at dimensions of less than 1 nanometer (one-billionth of a meter). Information at this level of detail can help researchers interpret experimental results and design future experiments.

Each shock-compression simulation ran for about 10 picoseconds (10-trillionths of a second), the approximate time it takes a shock wave to traverse a single ice grain in a comet. Even with the enormous capabilities available at Livermore's Terascale Simulation Facility, the researchers needed several months of computing time to calculate the first set of results. They found that a high degree of chemical reactivity occurred during the simulation, and aside from small amounts of water and ammonia, almost none of the starting materials remained at higher pressures and temperatures. The simulated reactions produced long, chainlike molecules with sequences of carbon–nitrogen bonds, which are required for both amino acids and proteins to synthesize. Says Goldman, "The quantity and complexity of carbon-nitrogen-bonded oligomers grew rapidly as the simulated pressure and temperature increased."

The team ran the simulation for an additional 30 picoseconds to observe the shock-compressed material as it cooled and expanded to atmospheric conditions. During this time, the carbon-nitrogen-bonded oligomers broke into simpler pieces, one of which was a precursor to the amino acid glycine. The expansion also produced hydrogen cyanide and formic acid, both of which are precursors to amino acid and complex organic synthesis. In other words, the team's



Physical chemist Nir Goldman is leading a computational research project at Livermore to simulate the materials that are synthesized when a comet impacts Earth.

results indicate that comets impacting Earth could have produced life-building molecules, which leads to the enticing thought that our progenitors just might have come from outer space.

Recent simulations have extended the timescales for shock compressions and expansions to nearly a full nanosecond, or a billionth of a second. These longer periods, Goldman notes, "will allow us to determine the chemical equilibrium products that can be produced during this type of impact event."

A Broader View

Livermore's Laboratory Directed Research and Development Program funded the initial work on this project. With support from the National Aeronautics and Space Administration's Astrobiology Program, the team is now exploring an array of scenarios, including a more direct cometary impact, resulting in even higher pressures and temperatures, and astrophysical ice mixtures with different chemical compositions. Perhaps the most exciting possibility to be considered is whether cometary impacts might have generated life on different celestial bodies, such as Jupiter's moon Titan, whose atmosphere has a density similar to that of Earth's.

"One interesting aspect of this work," says Goldman "is how applicable it is to the Laboratory's mission. Much of Livermore's research examines situations in which high pressures and temperatures are at work and result in novel chemical reactions. By learning more about chemistry under extreme thermodynamic conditions, we are making important contributions to many program areas around the Laboratory."

—Katie Walter

Key Words: amino acid chains, cometary compression, low-angle comet, molecular-dynamics simulation.

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